6. Vadose Zone Module

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The vadose zone is the hydrogeologic region that extends from the land surface to the regional water table (DOE/RL 1998b; Looney and Falta 2000). The goal of the Vadose Zone Module is to understand the transport and fate of contaminants as they move through the vadose zone. Thus, the principal geographic focus of this module is on areas at the Hanford Site that (1) underlie liquid waste disposal sites, (2) underlie underground storage tanks or solid waste burial grounds that have the potential for leaks and leaking, and/or (3) have experienced past leaks and spills.

The area between the surface of the land and the water table is called the vadose zone.

Results

Preliminary vadose zone results from the initial assessment are available for 25 different realizations of 9 different contaminants released from 533 different locations. This equates to a total of 179,750 individual simulations. Direct analysis of individual simulation results is impractical, so a flexible data extraction tool (VZGRAB) was used to view results from a number of perspectives.

At the highest level of analysis, total Hanford releases from the vadose zone were summed over all 533 sites by year, contaminant, and realization. Figure 6.1 depicts the predicted composite releases from one simulation (a run using the median value for all variables) for various contaminants over the entire Hanford Site. This result suggests that nearly all contaminant release rates peak and begin to decline prior to 1990. Carbon tetrachloride and chromium, continue to release for some time. (Note that releases for these chemicals are on a different scale – kilogram versus curie). Figure 6.1 also shows a secondary tritium peak in the 2020 to 2030 time frame in response to the sluicing of tanks and processing of the tank waste.

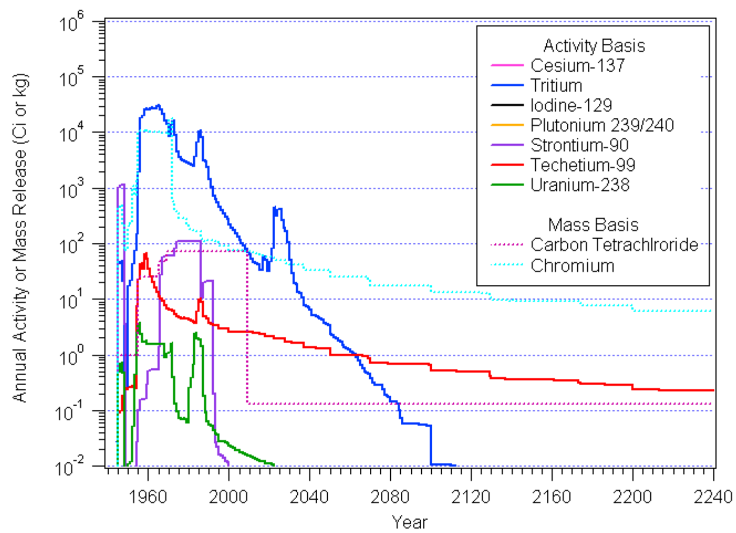

Figure 6.1. *Composite vadose zone releases to the groundwater of various contaminants from the median value.*

Figure 6.2 illustrates the predicted composite tritium releases from the vadose zone to the groundwater for all 25 realizations. Operation eras associated with World War II, the Cold War, and the restart of the PUREX Plant in the mid-1980s are apparent, as is a period of tank waste processing ending in 2028.

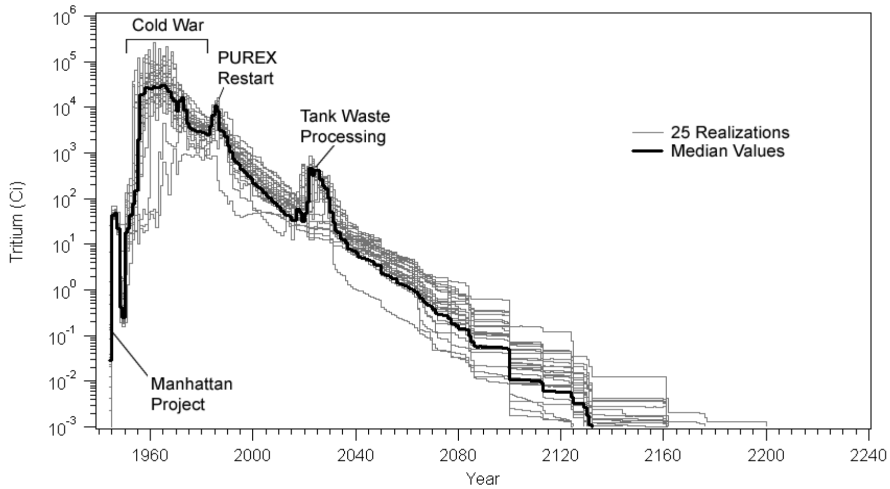

Figure 6.2. *SAC simulation (25 realizations) of total Hanford annual releases of tritium from vadose zone to groundwater. (Note difference in scale from Figure 6.1).*

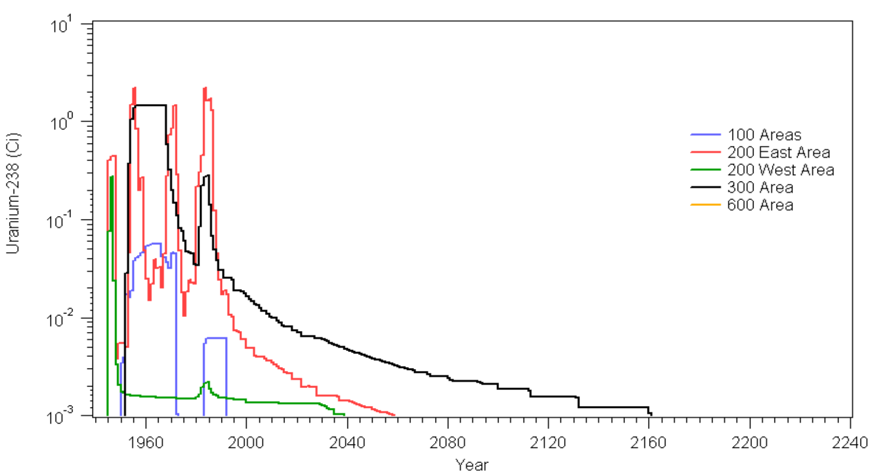

Figure 6.3. *Predicted composite uranium-238 releases to groundwater from different operational areas, simulation 5.*

At an intermediate level of analysis, mass balance and vadose zone releases to groundwater were summed by operational area. For example, Figure 6.3 illustrates that the predicted composite releases from the median value run for uranium-238 from the vadose zone to the groundwater are probably from the 300 and 200 East Areas .

Detailed analyses also were conducted at the site-specific scale for a single contaminant to examine how well the predictions matched the historical data, and to get some feeling for the degree of uncertainty between the various simulations. Overall, the vadose zone simulation results appear reasonable. Results suggest that the simulations generally match the location of the more mobile contaminants, but under-predict the depth of the less mobile contaminants. An example comparison of predicted cesium-137 concentrations beneath the 216-B-36 crib with those measured via spectral gamma logging in 1997 is shown in Figure 6.4.

High discharge volume sites such as cribs, ponds, and ditches pose some unique problems, particularly in trying to account for lateral spreading with a one-dimensional model. Thus, at some of these high volume sites, future revisions to SAC may examine the potential to incorporate the multi-dimensional aspect of horizonal fluid and contaminant spreading. The one-dimensional model used in the initial assessment for the vadose zone was configured only for aqueous phase transport; thus, the carbon tetrachloride simulations were conducted in a very simplified manner (i.e., as solubility and desorption controlled releases immediately above the water table). Incorporation of, and/or bench marking against, a multiphase model is recommended for future revisions. Additionally, the predictions for some mobile constituents discharged to some low volume sites (e.g. specific retention trenches), appear to suggest very rapid release to the groundwater (i.e. within the first year) — far sooner than could be expected from field data. Thus, additional study of past monitoring data and more detailed site-specific characterization and modeling efforts are needed to provide the ground truth data against which to assess the accuracy of these predictions and the veracity of underlying conceptual models. Other concerns that have risen from these results suggest that the hydraulic and/or retardation property distributions (and/or discretization of the vadose zone geology) may not be as representative as needed and/or that more robust models that can account for lateral spreading are needed to more closely match the peak concentrations and locations of the predictions with those of the actual field data.

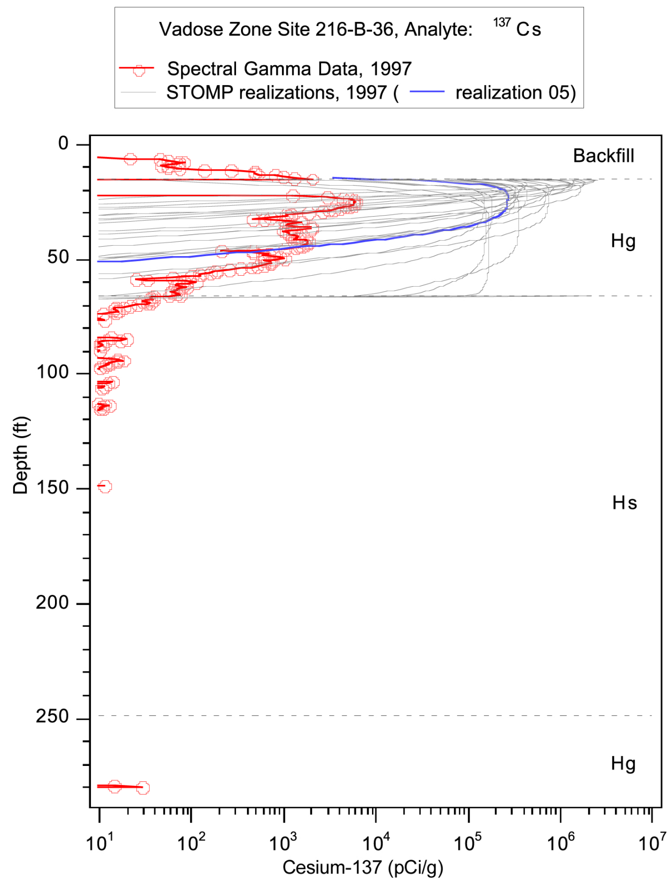

Figure 6.4. *Comparison of predicted cesium-137 concentrations beneath the 216-B-36 crib with those measured via spectral-gamma logging in 1997.*

Conceptual Model

Looney and Falta (2000) describe a conceptual model as a detailed technical description of the system, that answers the question "how do we believe the system actually operates?" Conceptual models are evolving hypotheses that identify the important features, events, and processes controlling fluid flow and contaminant transport at a specific field site and in the context of a specific problem.

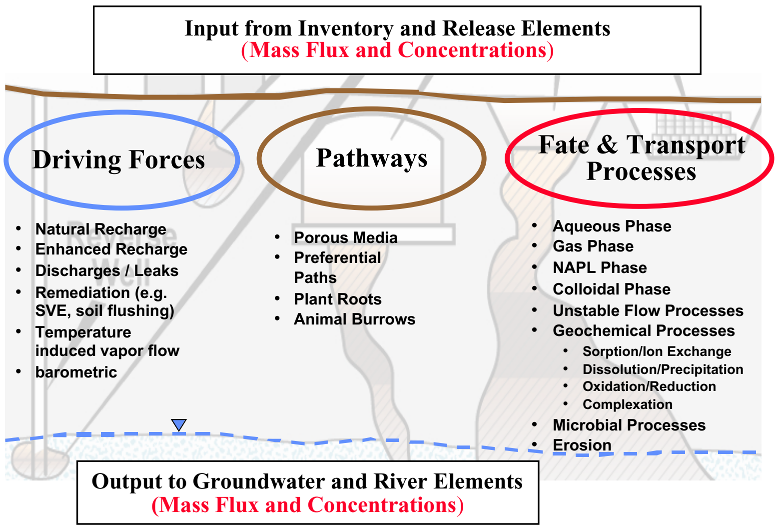

Figure 6.5. *Some primary conceptual model components for flow and transport of contaminants through the vadose zone.*

Vadose zone contamination is primarily the result of waste effluent releases to liquid waste disposal facilities, leakage from retention basins, and to a lesser degree by accidental releases of contaminants through low-volume spills, and dry waste burial grounds. Billions of liters of wastewater have created large contamination plumes within the vadose zone. Figure 6.5 illustrates the conceptual model from the Vadose Zone.

The primary driving forces for contaminant transport are the source/release events, and recharge events. The dominant transport pathway is downward through the vadose sediments. Stratigraphic layering, variations in the hydraulic properties, and the presence of impeding features (e.g. caliche layers) can locally alter and redirect the movement of contaminants laterally. Discordant features (either natural or manmade – e.g. clastic dikes, fractures, unsealed bore-holes) can provide preferential pathways capable of concentrating or contributing to phenomena such as fingering and funnel flow. Wilson et al. (1995) describes flow within the vadose zone as dynamic and characterized by periods of unsaturated flow at varying degrees of partial saturation punctuated by episodes of preferential, saturated flow in response to hydro-logic events or releases of liquids.

The movement of contaminants in the vadose zone is affected by their sorption in the far field, and sometimes by complex dissolution/precipita-tion reactions between the waste liquids of extreme pH and the slightly alkaline sediments in the near-field. The significance of sorption is that it delays downward movement of the contaminant and allows degradation processes (e.g. radioactive decay) to occur and for some contaminants, rather irreversible incorporation into the sediment. The sorptive capacity of the vadose zone sediments is fairly high, however the amount of sorption is a function of many factors, including mineral surface area and type, con-taminant type (speciation) and concentration, overall solution chemistry and concentration, and reaction rates for the control adsorption or precipi-tation, dissolution, and hydrolysis reactions. Some contaminants do not sorb at all and are moved along with the bulk solution.

Contaminants that exist in the gas phase (e.g. carbon tetrachloride) are subject to atmospheric venting. Contaminants too near the soil surface are subject to animal and plant uptake. Contaminants that are consumed by microbes are subject to degradation into other compounds that may or may pose a risk to humans and the environment.

The Vadose Zone Module focuses on areas at Hanford that underlie liquid waste disposal sites and tanks, have experienced leaks, or have the potential for leaks.

DOE (1999d) summarizes the state of knowledge concerning characterization, modeling, and monitoring of the vadose zone. The *Candidate Sets Report* (http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm), the *Preliminary System Assessment Capability Concepts for Architecture, Platform and Data Management* (http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm) and Soler et al. (2001) provide a compilation of the

- features (the structure and transport properties of the various pathways)
- events (e.g. recharge, source releases)
- processes (the fate and transport processes/mechanisms, including driving forces of precipitation and net infiltration)

considered relevant to contaminant flow and transport within the vadose zone beneath the Hanford Site. Last et al. (2001) illustrate these major processes via a master process relationship diagram.

Specific topics of interest to the Hanford Site include:

- subsurface contamination (i.e. characteristics of past disposal and leak age, including chemistries, volume, and distribution)
- surface hydrologic features and processes (e.g. winter rain and snow melt, water line leaks, infiltration, deep drainage, and evaporation rates)
- subsurface geologic and hydraulic features and processes (e.g. stratigraphy, structures, physical properties, geochemistry, and microbiology of the sediments above the water table) (DOE/RL 1999b).

Implementation Model

The SAC model is being developed to assess the cumulative impact of radioactive and chemical waste at the Hanford Site. The vadose zone element relies on input from the inventory and release elements. This

Some dissolved elements move freely through sediment while others tend to bind to sediment grains. This tendency to bind to sediment is expressed as a K_d value. The higher the K_d value, the more the element binds to soil.

needed input includes the spatial and temporal distributions of waste releases and the mass flux and concentrations of these releases.

The large scale and complexity of a sitewide cumulative assessment together with the complex behavior of contaminants through the vadose zone and the many unresolved issues and levels of uncertainty, necessitates simplification of the site features, the release events, and the contaminant fate and transport processes.

Due to the computational complexity and time requirements of more complex modeling options, a simplified conceptual model was selected for the initial demonstration (see *Preliminary System Assessment Capability Concepts for Architecture, Platform and Data Management* [http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm]). Implementation of this conceptual model is schematically illustrated in Figure 6.6.

Inputs to the model come primarily from the inventory and release elements, including recharge, and the mass flux and concentrations of the selected constituents. Other inputs include the effectiveness and timing of remedial actions that might either reduce the mass and/or concentration of contaminants in the vadose zone, or might reduce the flux of deep infiltrating moisture (i.e. capping). These inputs include infiltration rates from both natural events (e.g. precipitation) and operational activities (e.g. excavation, capping). Each site is represented by a few major hydrostratigraphic units that are of uniform thickness, horizontal, homogeneous and isotropic (see Figure 6.6). Hydraulic and geochemical parameters for each hydrostratigraphic unit are represented by stochastic distributions reflecting the uncertainty in measured properties. Definition of the hydrostratigraphy and the associated hydraulic, transport, and geochemical properties of the one-dimensional soil column were based on existing geologic, soil physics, and geochemical data bases (*Vadose Zone Data Gathering Report* [http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm). Distribution coefficient (K_d) values were selected

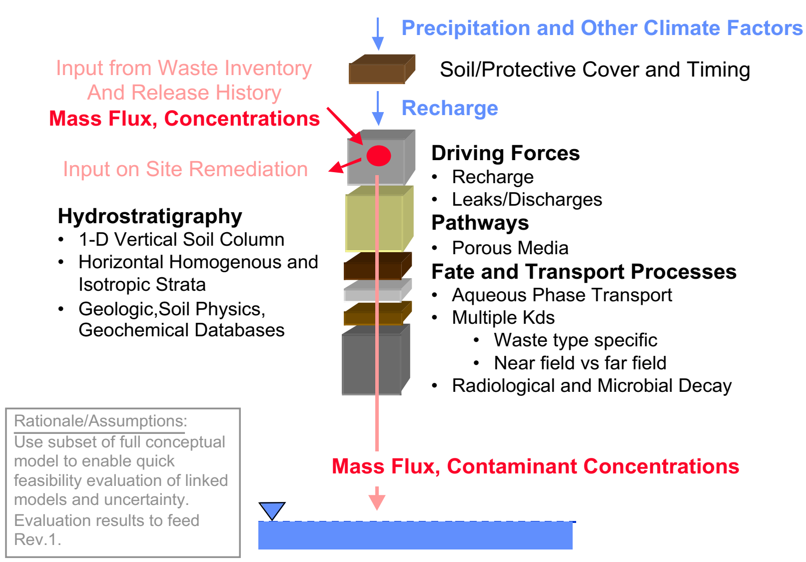

Figure 6.6. *Primary components/factors incorporated into the simplified implementation model.*

based on the soil type, waste type, and analysis of existing vadose zone plumes in both the near, intermediate, and far field – recognizing the effects of highly concentrated complex waste chemistries on the mobility of contaminants.

The transport pathway to be simulated is aqueous phase transport through the porous media of the vadose zone. Radiological decay is simulated using first order decay models. Sensitivity and uncertainty analyses are used to capture some effects of model simplification. Within the vadose zone, uncertainty (i.e., probability distribution functions) is assigned to waste discharge rates, hydraulic properties, geochemical retardation, and transport parameters. This approach quantifies the uncertainty in a single conceptual model of vadose zone contaminant transport. Future revisions to SAC may address the uncertainty associated with natural and artificial recharge and multiple conceptual models.

Output from the vadose zone element feeds the groundwater and/or the risk elements. This output is primarily in the form of spatial and temporal distributions of the mass flux and concentration of contaminants.

Numerical Model

Kincaid et al. (2000) identified the Subsurface Transport Over Multiple Phases (STOMP) computer code (White and Oostrom 1996) as the code for the Vadose Zone Flow and Transport Module for SAC.

The initial assessment simulates intentional and unplanned liquid discharges and solid waste disposal to 890 individual sites but aggregates 200 solid-waste burial grounds and unplanned releases into 30 aggregate sites based on their location, waste release model, and waste chemistry designations. These and other aggregations yield a total of 533 sites to be individually simulated. These sites were grouped into 13 different hydro-geologic provinces (or aggregrate areas; Figure 6.7), each represented by a single generalized one-dimensional vadose zone profile.

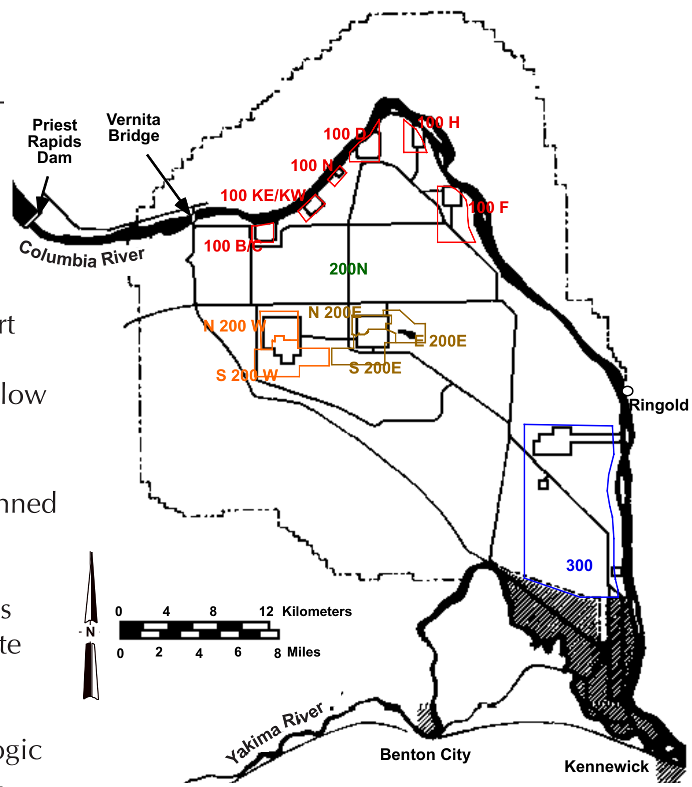

Figure 6.7. Location of aggregate areas to be represented by a single generalized stratigraphic column.

A series of 64 base templates were identified for application in 13 hydrogeologic provinces. These base templates consist of the one-dimensional stratigraphy, hydrologic properties, and geochemical properties as well as the waste site type (e.g., crib, tank, etc.) and waste chemistry designation. Each individual template was configured with the hydraulic and geochemical parameters necessary for STOMP to simulate the flow and transport through the vadose zone. A more complete discussion regarding the development of the 64 base templates is provided in the *Vadose Zone Data Gathering Report* (http://www.bhi.erc.com/projects/vadose/sac/sacdocs.htm). The hydraulic and geochemical input parameter described in this report were updated/revised prior to running the final version of the initial assessment.

This approach (and the rationale behind it) for modeling contaminant transport through the vadose zone for SAC is presented in *Preliminary System Assessment Capability concepts for Architecture, Platform and Data Management* (http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm). This approach uses base templates to represent the vadose zone beneath all waste sites within a given hydrogeologic province. However, the actual simulation of each waste site assigned to a given template is implemented at the individual waste site's centroid coordinates.

*Some cesium is naturally present in the environment. However, **cesium-137** is a radionuclide in spent nuclear fuel and radioactive waste resulting from the operation of nuclear reactors and fuel reprocessing plants. Cesium-137 has a half-life of 30 years and should naturally decay in a relatively short time. In addition, cesium is not very mobile in Hanford vadose zone and groundwater sediments. At the time the initial assessment was designed, cesium mobility was being studied because it had been discovered at significant depths beneath single-shell tank leak locations. For these reasons, it was included as an example of a moderately sorbing and decaying contaminant in the list of contaminants for the initial assessment.*

Once each site was assigned to a hydrogeologic province and a representative base template, site-specific parameters such as the site location (centroid), and recharge rates based on surface cover changes were added. Each site, either a separate liquid disposal site or an aggregation of several solid waste burial ground or unplanned release sites, was then assigned a unique alphanumeric identifier.

History Matching

The vadose zone simulation results appear reasonable based on vadose zone and groundwater history matching exercises. Initial comparison of simulation results against vadose zone field data was completed for 13 different sites. These sites represented (1) facilities from different aggregate areas, (2) facilities with a range in discharge from low volume (216-B-46 crib) to high-volume (216-A-8 crib), (3) facilities that received chemically different waste streams, (4) facilities that received at least one of the selected constituents of interest defined in Kincaid et al. (2000) and, most importantly, (5) facilities for which historical contaminant distributions through time were available. These comparisons were primarily conducted deterministically using the average, median, and/or best estimate values for hydraulic and geochemical parameters (details on the physical and geochemical parameters defined for the vadose zone templates used in these simulations can be found in *Vadose Zone Data for Initial Assessment Performed with the System Assessment Capability,* http://www.bhi-erc.com/projects/vadose/sac/sacdocs.htm), and wetted column areas that varied as a function of the facility footprint (e.g., 1, 2, or 3 times the facility footprint area).

The results from the Vadose Zone Module appear reasonable when compared to historical data.

A limited number of history matching cases also were conducted in a stochastic mode to develop an understanding of the resulting distributions. The high discharge volume sites such as cribs, ponds, and ditches pose some unique problems, particularly in trying to account for lateral spreading with a one-dimensional model. The results of the first runs performed with SAC were presented to the Integration Project Expert Panel in September 2001. Analysis performed on these early results identified a number of issues that needed to be addressed before the tool could be considered useful. The major vadose zone issues were addressed by replacing a simple algorithm for assigning the wetted column area, with the capability to calculate the wetted column area based on unit-gradient approach. During fall 2001, the SAC model was changed to estimate the wetted column by determining the area needed to pass the vadose zone flux through the lowest hydraulic conductivity (lowest K_{SAT}) valued hydrogeologic layer. Hydraulic and geochemical input parameters were also updated at this time. Limited history matching of results using the lowest K_{SAT} model also appear to be reasonable for mobile constituents at most sites when compared to the historical groundwater data. However, at some sites (e.g. BC cribs and trenches) the arrival of mobile species to the water table was much sooner than field data suggest. Also, for at least some of the less mobile species such as cesium-137 at high volume sites, future revisions to SAC should have the potential to incorporate multi-dimensional aspects of vadose zone fluid flow and the kinetics of contaminant transport.

The one-dimensional model used in the initial assessment was configured only for aqueous phase transport; thus, the carbon tetrachloride simulations were conducted in a very simplified manner (i.e., as a solubility and/or desorption controlled release at the water table). Incorporation of, and/or bench marking against, a multiphase model is recommended for the next revision of SAC.

The predictions for some mobile constituents discharged to some low volume sites (i.e., specific retention trenches), appear to suggest very rapid release to the groundwater (i.e., within the first year) — far sooner than previously expected based on the accepted conceptual model for retention trenches. These results suggest that the hydraulic and/or retardation property distributions may not be as representative as needed, and more robust models that can account for lateral spreading may be needed. Therefore, additional study of past monitoring data and more detailed site-specific characterization and modeling efforts are needed to provide the information against which to measure the accuracy of these predictions and the veracity of the conceptual model in the initial assessment.